## Unusual Parallel Entanglement of Metal-Organic 2D Frameworks with Coexistence of Polyrotaxane, Polycatenane and Interdigitation

Xin-Yi Cao,<sup>[a]</sup> Yuan-Gen Yao,\*<sup>[a]</sup> Stuart R. Batten,\*<sup>[b]</sup> En Ma,<sup>[a]</sup> Ye-Yan Qin,<sup>[a]</sup> Jian Zhang,<sup>[a]</sup> Rui-Bo Zhang,<sup>[a]</sup> and Jian-Kai Cheng<sup>[a]</sup>

- [a] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China
- [b] School of Chemistry, Monash University, Victoria, 3800, Australia

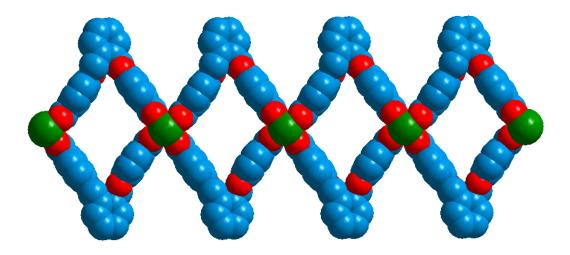


Figure S1 Space-filling plots of the neutral chain of loops  $[Zn_2(1,2-BBOMB)_2]_n$  in compplex 1.

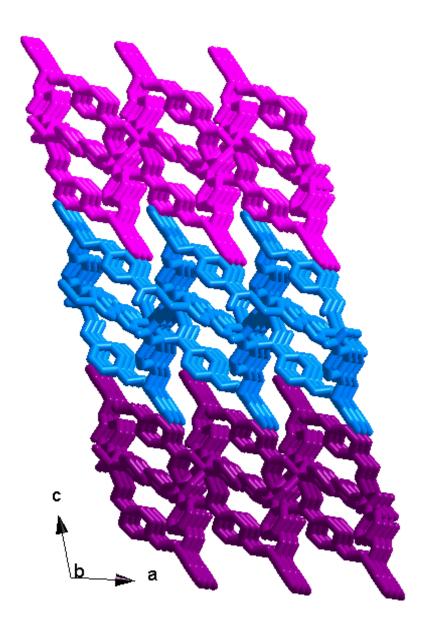


Figure S2 The adjacent layers are interdigitated each other to form 3D architecture in complex 1.

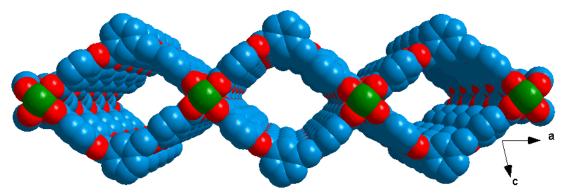


Figure S3 Space-filling plots of the single net in  $\mathbf{2}$  viewed along the b axis.

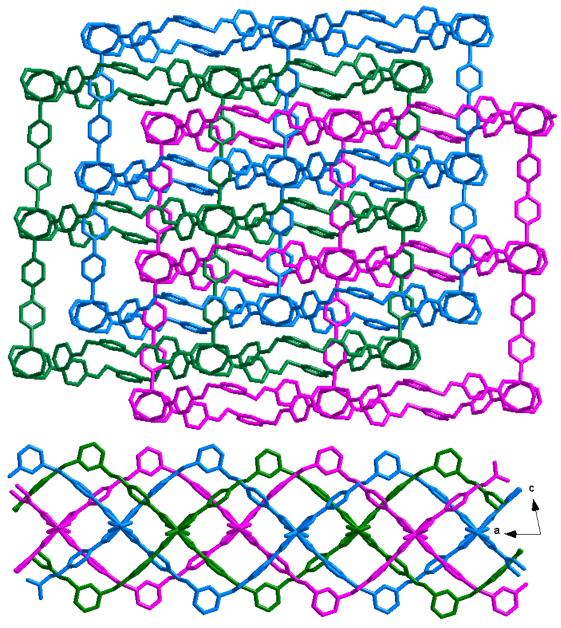


Figure S4 Two views of parallel 2D→2D triply interpenetrating nets in 2

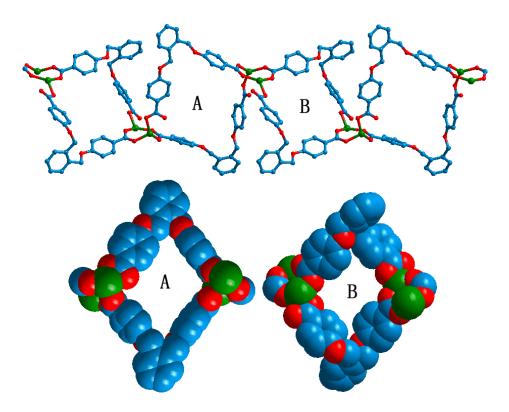


Figure S5 A view of the neutral chain of loops  $[Zn_2(1,2-BBOMB)_2]_n$  with two type rings in compplex 3. Space-filling plots of type A and B loops in 3.

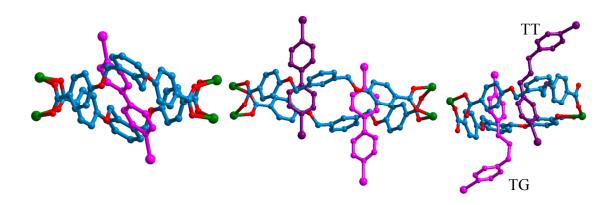


Figure S6 The comparison of the stereochemical relationships between the 4,4'-bipy or bpp rods and the [Zn<sub>2</sub>(BBOMB)<sub>2</sub>] loops through which it passes for complexes 1 (left), 2 (middle) and 3 (right).

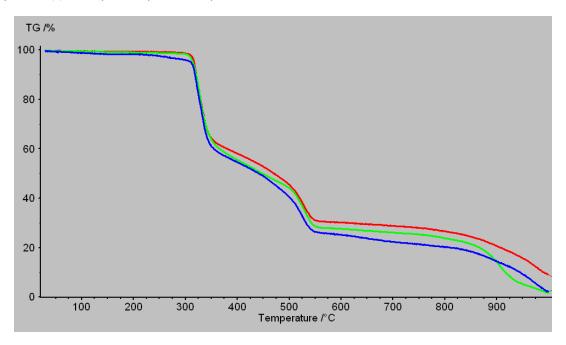


Figure S7 TGA curves for complexes 1 (red), 2 (blue) and 3 (green).